Frank Laboratory of Neutron Physics
Joint Institute for Nuclear Research

Transport Simulation of Very Cold Neutrons in Nanodiamond Powders

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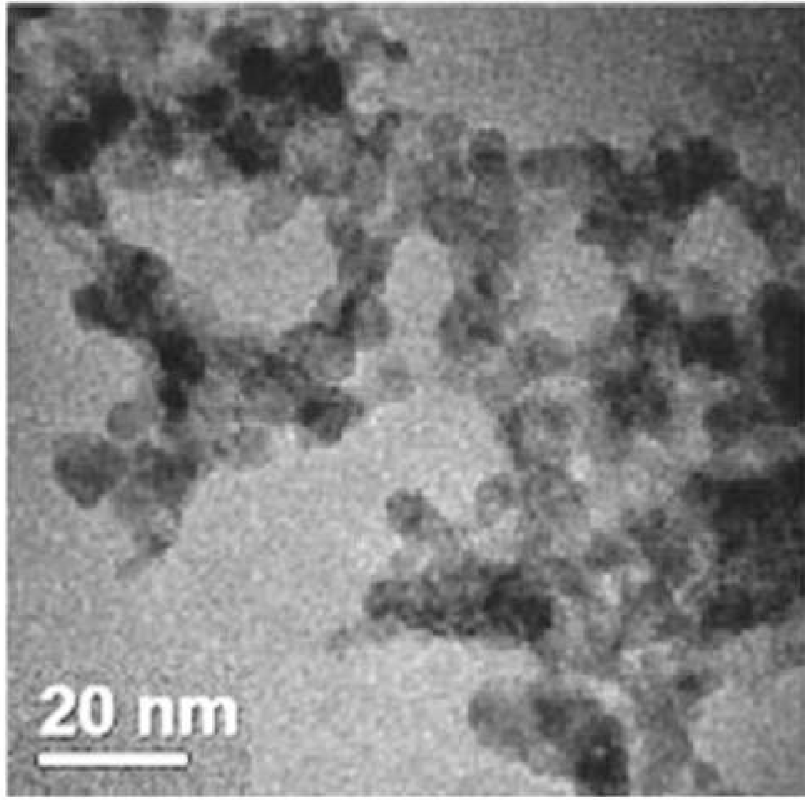
UCN **VCN** CN

- the typical wavelengths are 2.5–60 nm;
- the velocities are 7–160 m/s;
- the energies are 0.25–130 μeV.

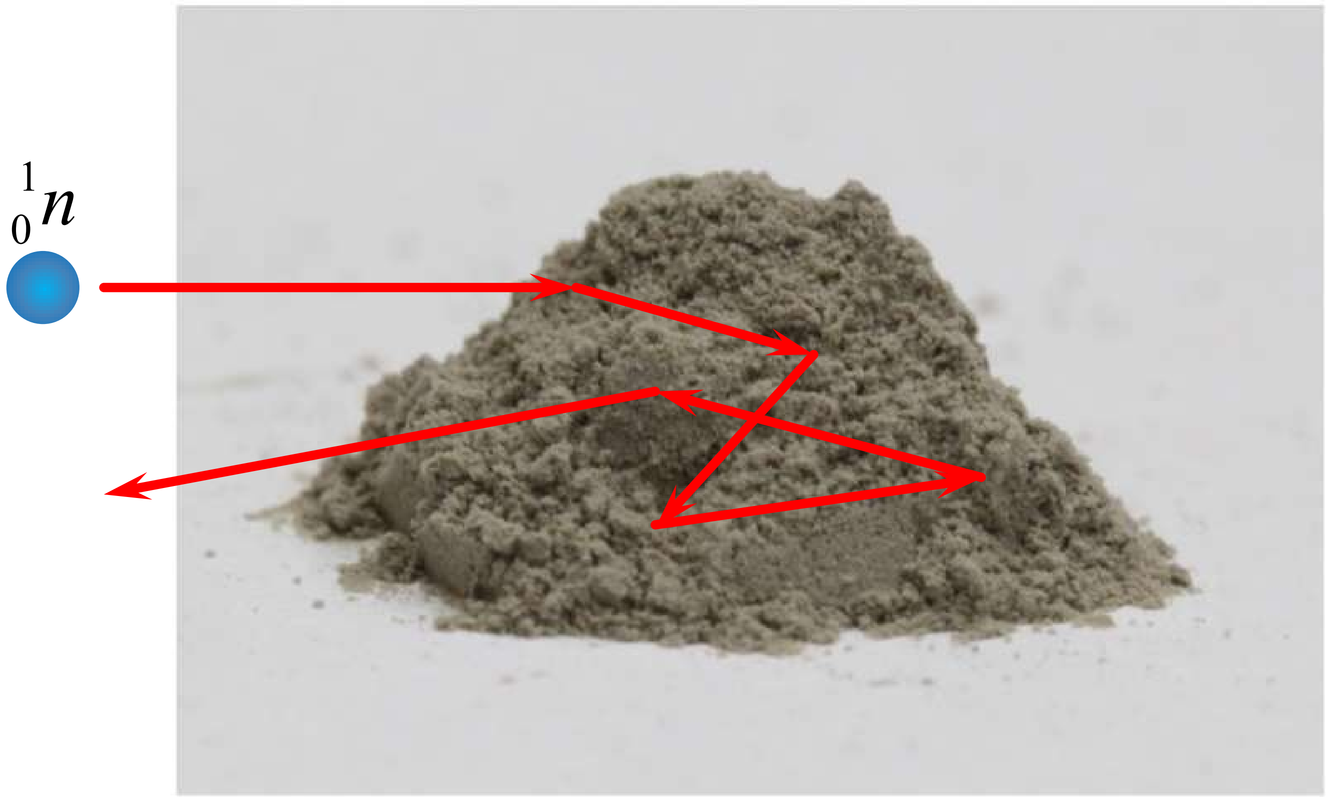
The advantages of VCN:

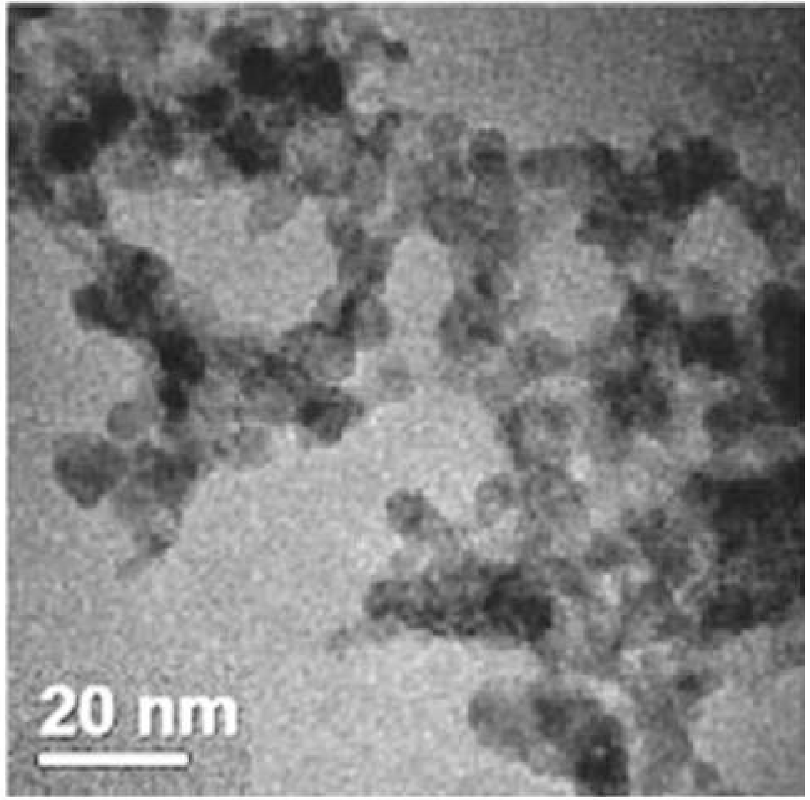
- long time of observation;
- large angles of reflections from mirrors;
- larger phase shift and as result more sensitive to contrast variation;
- large coherent length;
- large capture cross-section and big contrast at transmission;
- possibility structure analysis of large molecular complexes; etc.

What is Nanodiamond Powder?



What is Nanodiamond Powder?





Artem'ev V.A. Atomic Energy **101**, 901 (2006)

The interaction with nanoparticle

The amplitude of neutron scattering on a round uniform particle in the first Born approximation:

$$f(\theta) = -\frac{2m}{\hbar^2} V R^3 \left(\frac{\sin(qR)}{(qR)^3} - \frac{\cos(qR)}{(qR)^2} \right), \quad q = 2k\sin(\theta)$$

$\boldsymbol{\theta}$ is the scattering angle,
m the neutron mass,
V the real part of the nanoparticle optical potential,
ħ the Planck constant, r the nanoparticle radius,
k=2π/λ the neutron wave vector,
λ the neutron wavelength.

The scattering cross section:

$$\sigma_s = \int |f|^2 \, d\Omega = 2\pi \left| \frac{2m}{\hbar^2} V \right|^2 R^6 \frac{1}{(kR)^2} I(kR),$$

where

$$I(kR) = \frac{1}{4}\left(1 - \frac{1}{(2kR)^2} + \frac{\sin(4kR)}{(2kR)^3} - \frac{\sin^2(2kR)}{(2kR)^4} \right)$$

$$\theta_{scat} \sim \lambda/d, \; d \gg \lambda$$

Nesvizhevsky V.V. Phys. At. Nucl. **65**, 400 (2002)

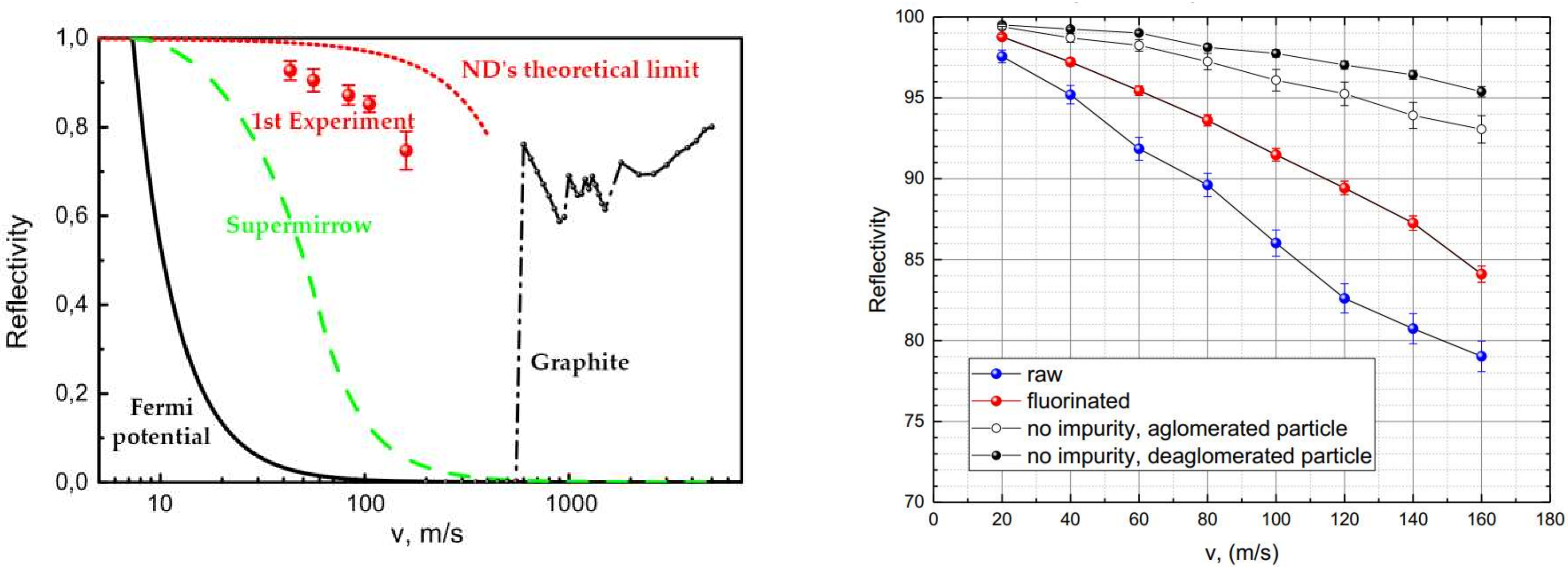
The goal is:

1. to maximize coherent scattering cross section σ_s ;
2. to minimize absorption cross section σ_a as much as possible.

For carbon:

σ_s = 5.551 barn

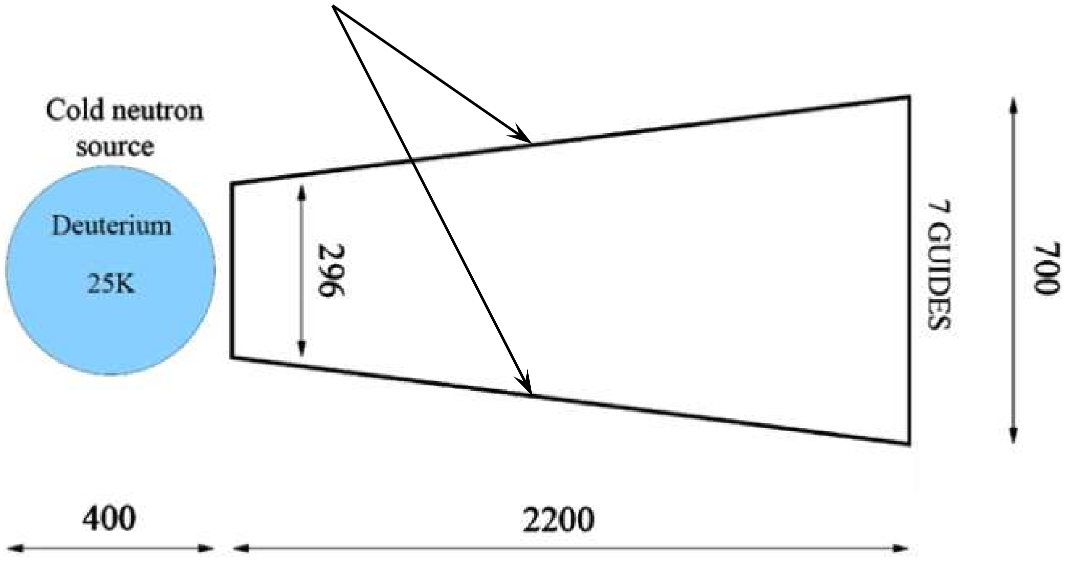
σ_a = 0.0035 barn



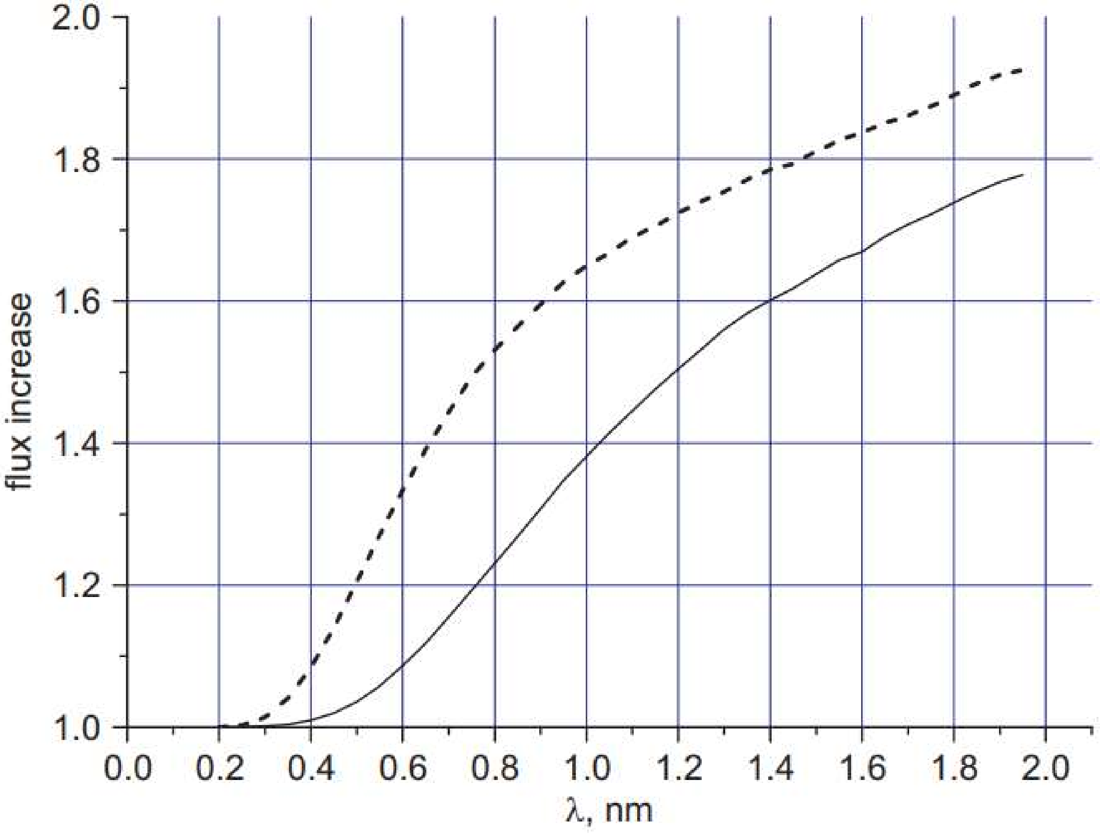
The elastic reflection probability for isotropic neutron flux is shown as a function of the neutron velocity.

Lychagin E.V. et al. Physics Letters B **679**, 186 (2009)

Nanodiamond covered walls,
d=5 mm

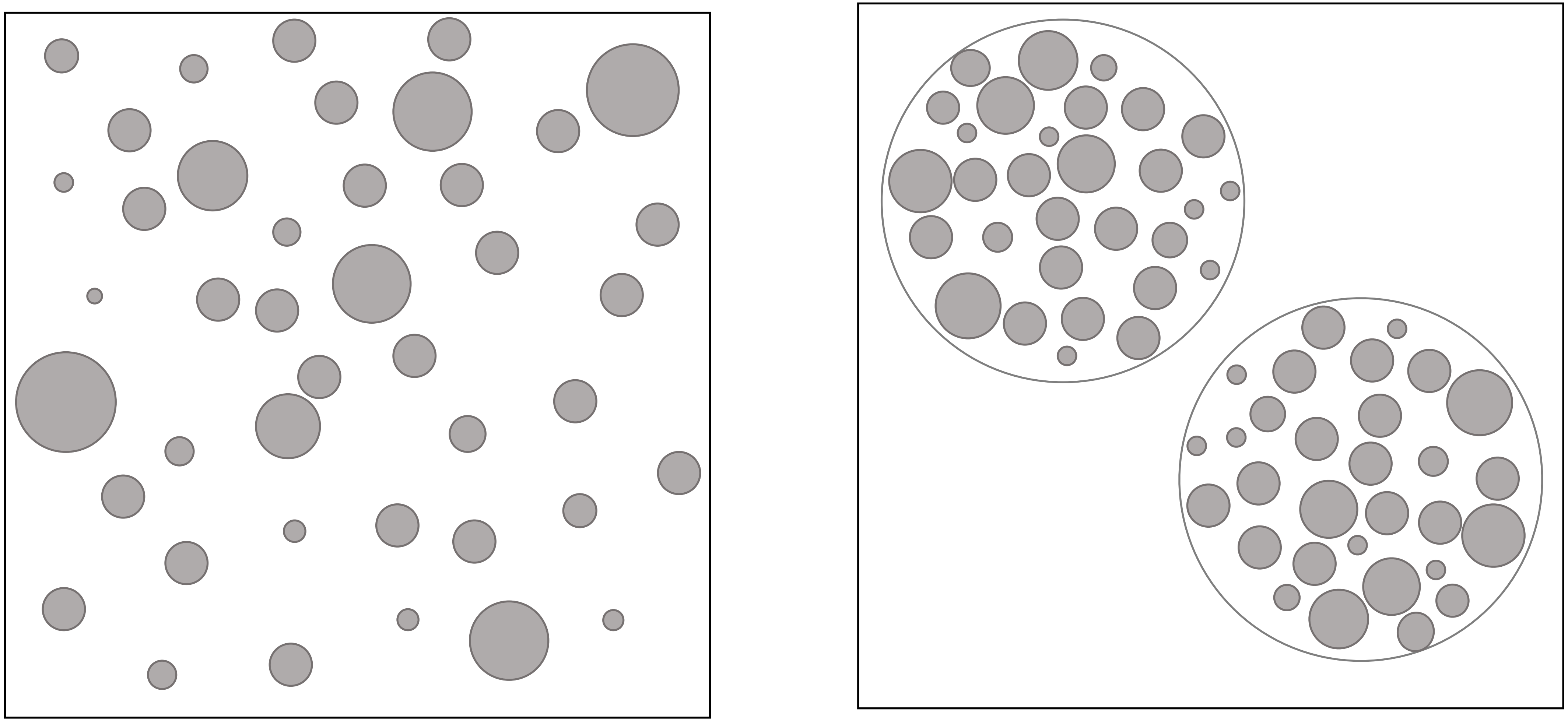


Geometry of a setup

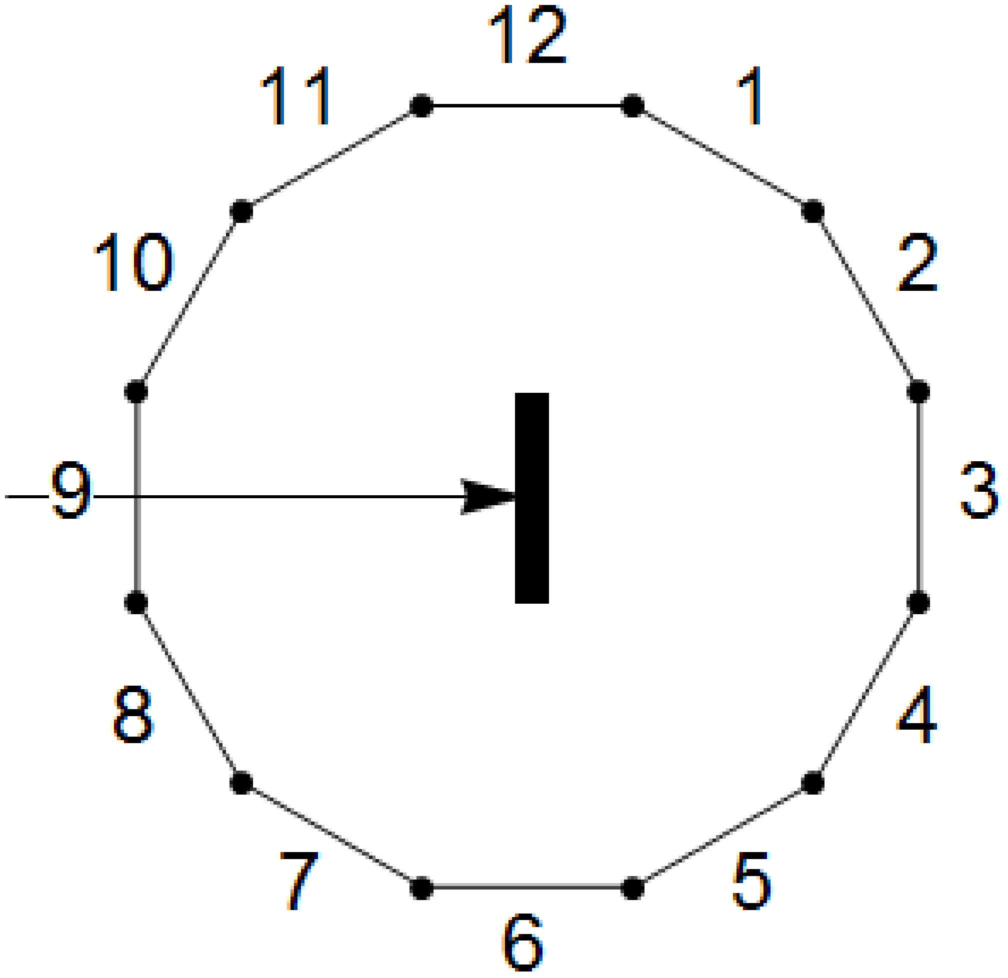


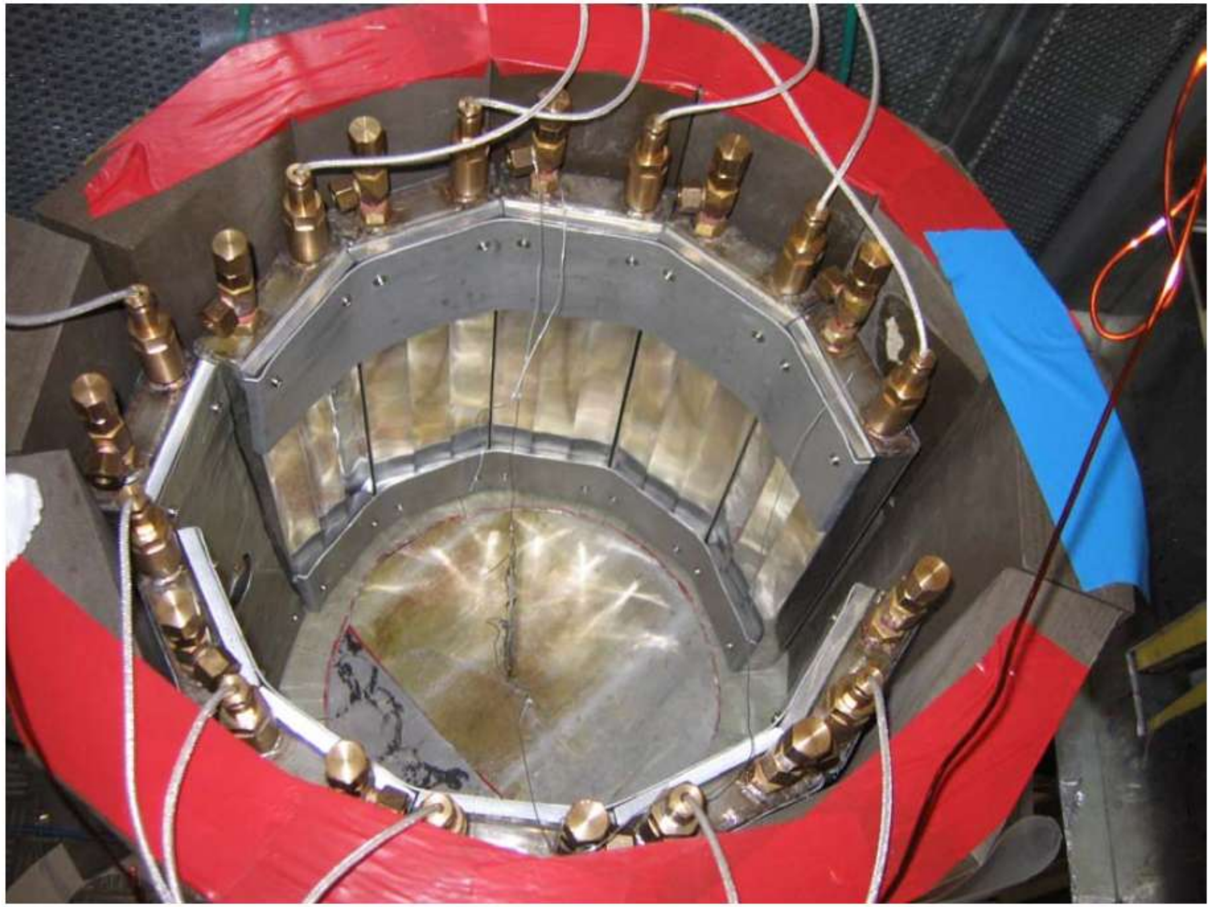
Increase in the neutron flux at the neutron guide entrance

Cubitt R. et al. Nucl. Instr. & Meth. A **622**, 182 (2010)



Two existing models: the model of free nanoparticles (left) and the model assumed the agglomeration of nanoparticles (right).

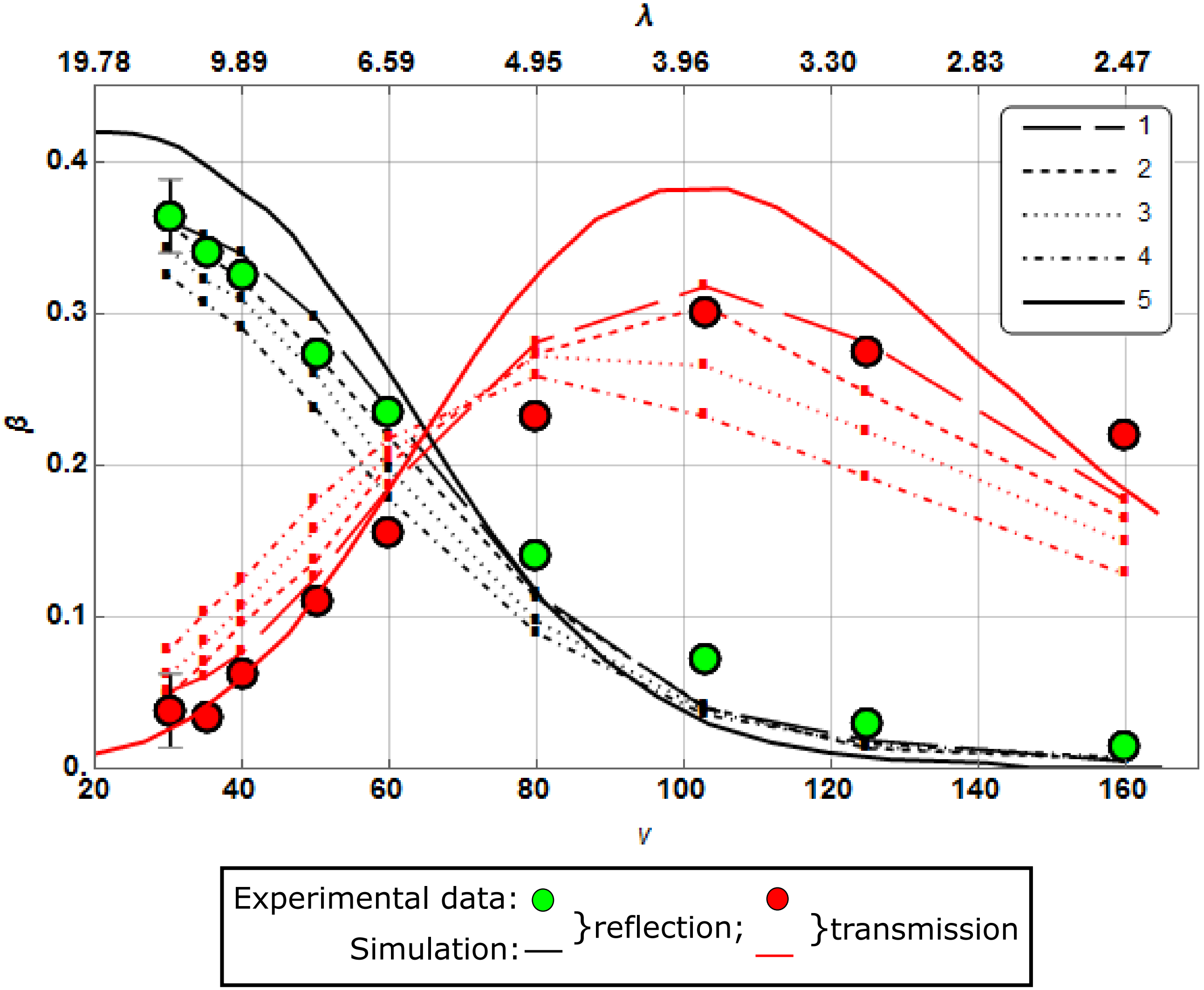




The layout of the plate, detectors and their numeration.

Nesvizhevsky V.V. et al. Nucl. Instr. & Meth. A **595**, 631 (2008)

Models comparison



Comparison of the probabilities β of neutron reflection (black) and transmission (red) in relation with the velocity v (m/s) and the neutron wavelength λ (nm).

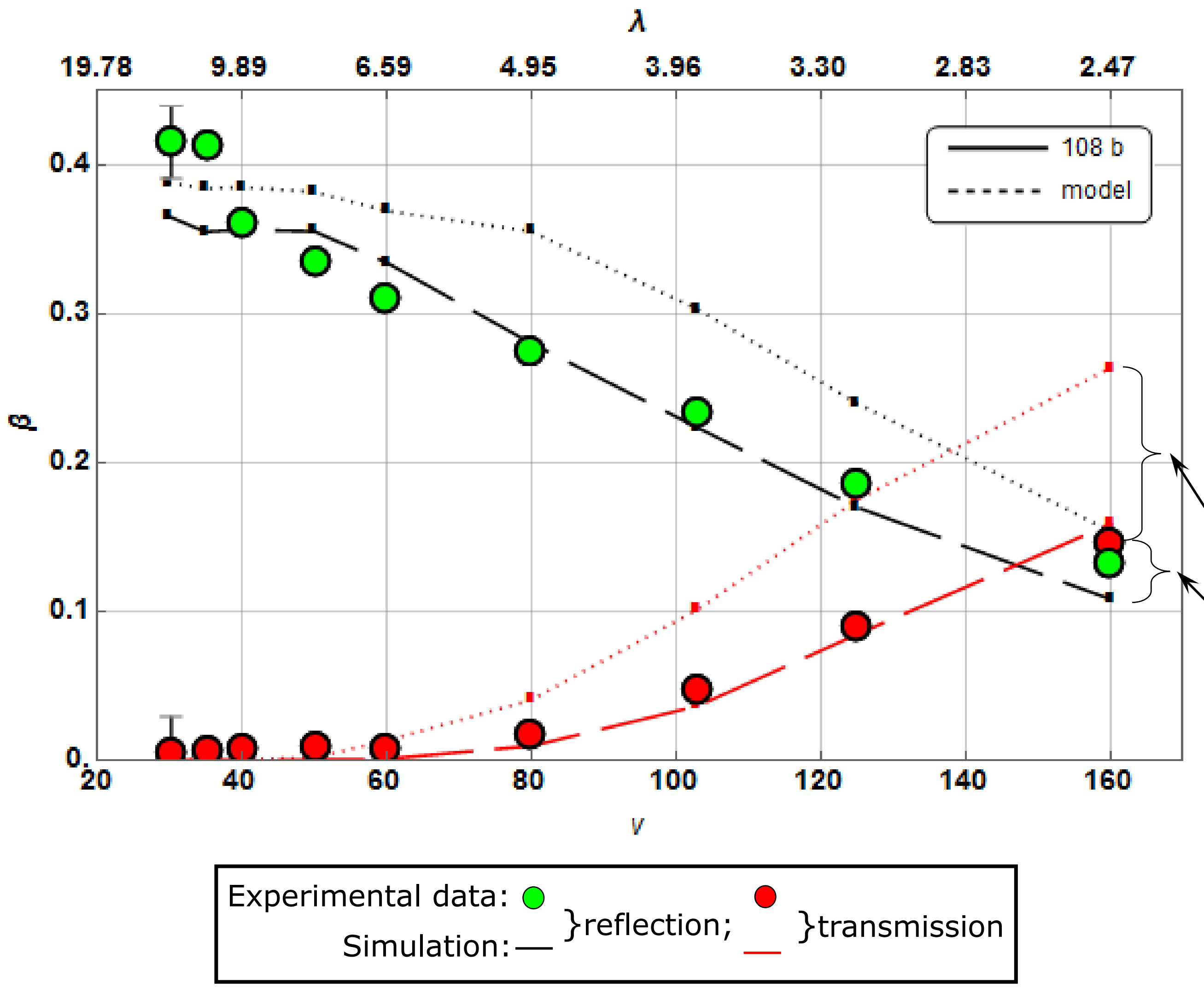
1–4 – accounts the effects of the medium density;

5 – the initial model of “free” nanoparticles.

$$1-\gamma = 0.523; 2-\gamma = 0.569;$$

$$3-\gamma = 0.625; 4-\gamma = 0.682.$$

Models comparison



Comparison of probabilities β of neutron reflection (green round points) and passage (red round points) in relation with the velocity v (m/s) and the neutron wavelength λ (nm).

Thickness of the nanopowder plate is 6 mm. $\gamma = 0.625$.

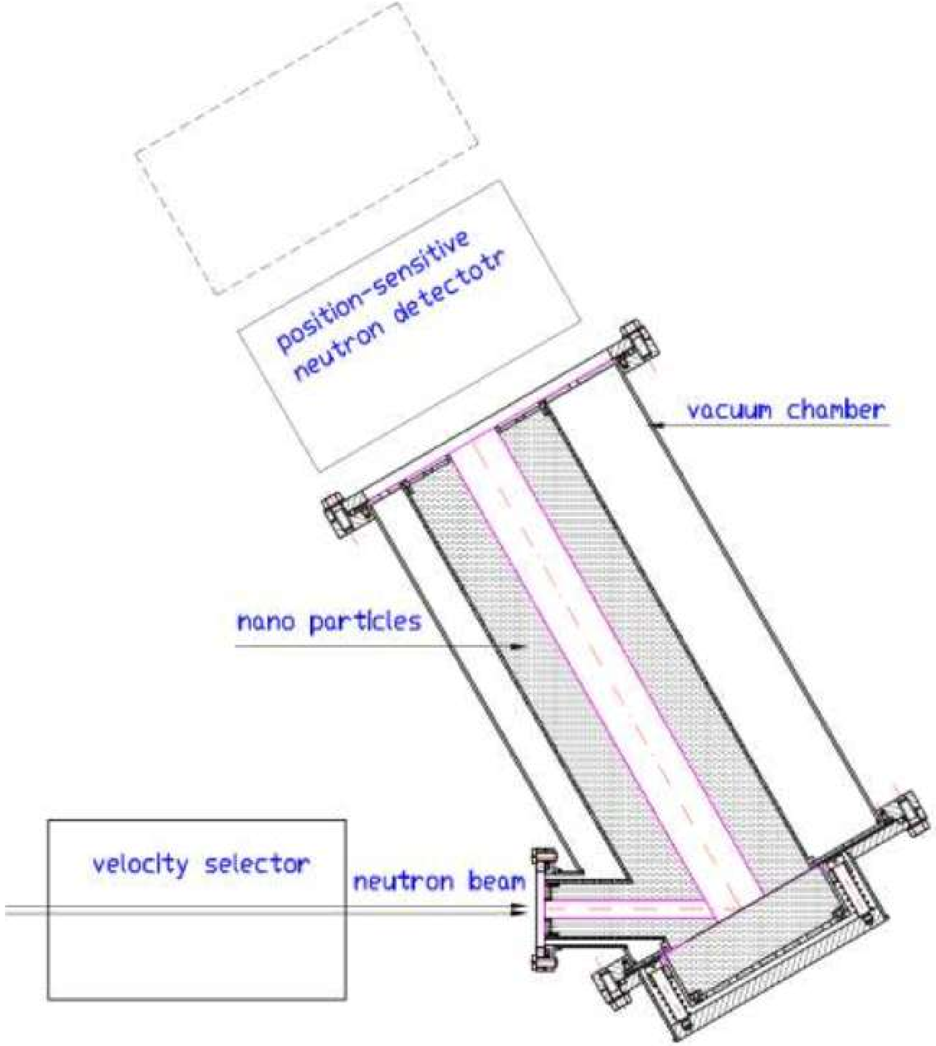
due to the $\sigma^{H}_{in.sc}$

Krylov A.R. et al., Crystallogr. Rep. **56**, 1186 (2011)

Fluorinated diamond nanopowder

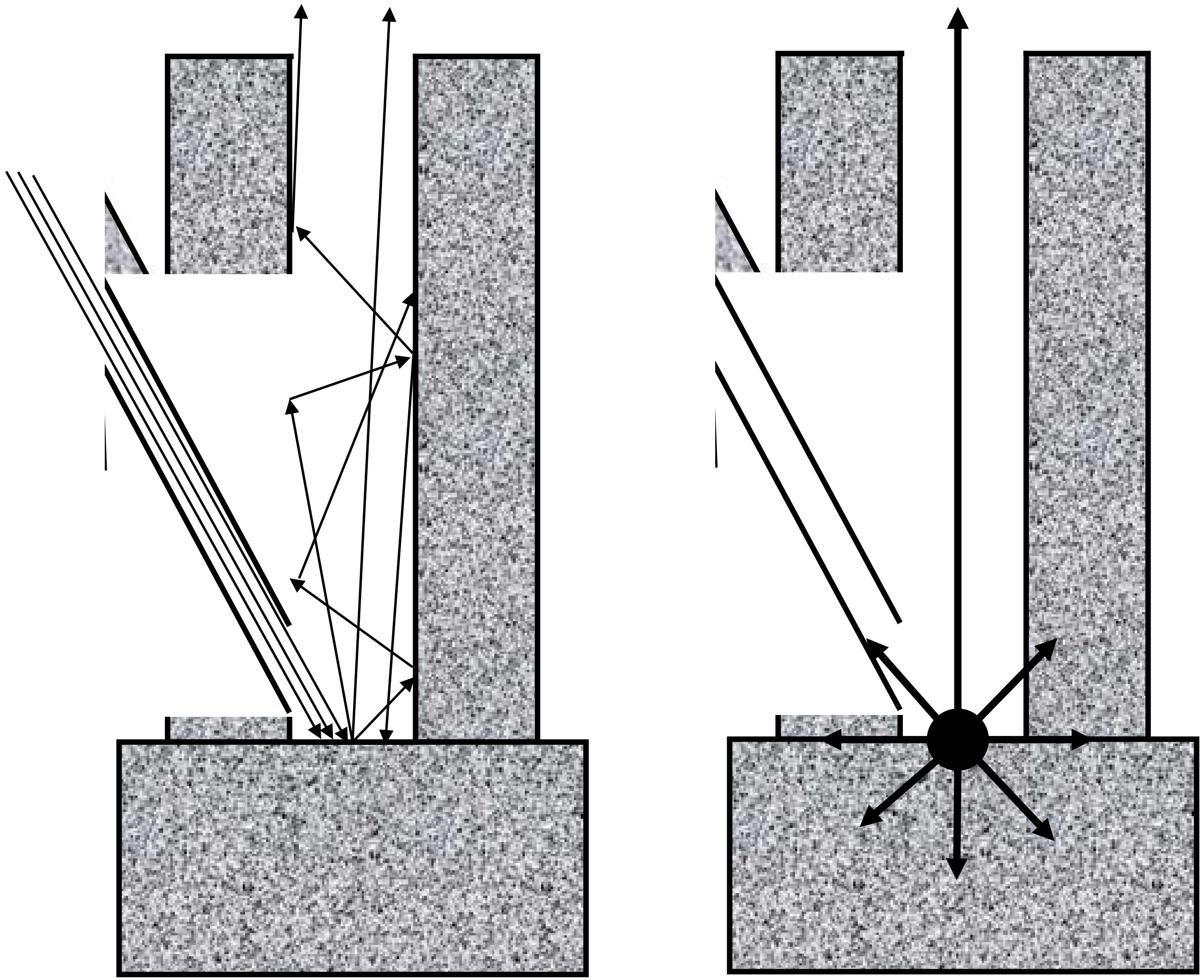
1. Hydrogen level was decreased from $C_{7.5\pm0.2}H$ to $C_{430\pm30}H$;
2. sp^2 carbon shells were destructed;
3. **Nanodiamond clusters were disaggregated;**
4. sp^3 diamond cores remained unaffected.

So, the next step was to try to increase the VCN flux (2017).



Nesvizhevsky V.V. et al., Carbon **130**, 799 (2018)

Fluorinated diamond nanopowder



Fluorinated diamond nanopowder

One of the goals was to find a suitable model for describing the experimental data.

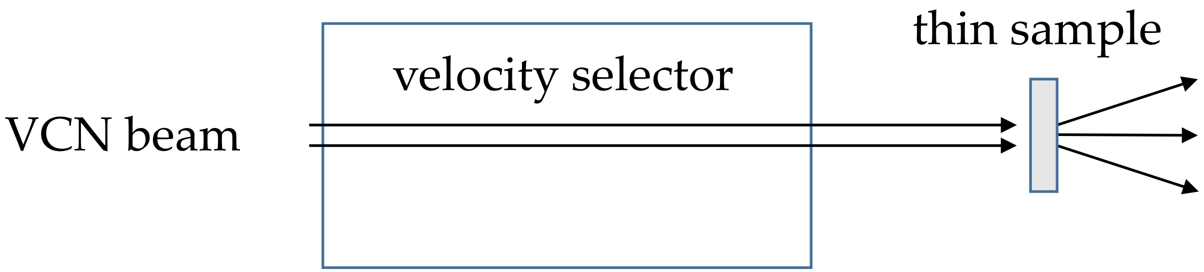
<u>An additional difference</u> from the raw nanopowder is that we still don't know much about the properties of the fluorinated diamond nanopowder:

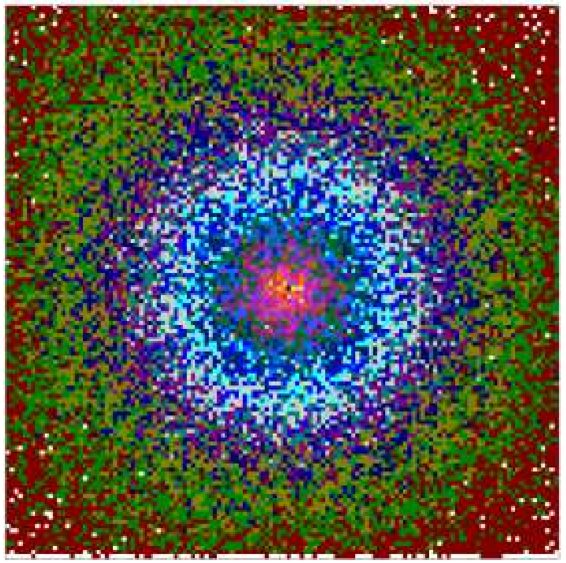
- the size distribution (cores and shells);
- elemental and phase compositions;

+ the average diameter is ~4.3 nm (via the Scherrer equation);
+ atomic concentration of metallic impurities.

Literature data about the detonation synthesis helped us to define the values of elemental and phase composition in narrow ranges. In turn, it allowed finding realistic combinations of shell properties and parameters of the size distribution described by, for instance, the log-normal or other laws.

Transmission of VCN


VCN beam
velocity selector
thin sample

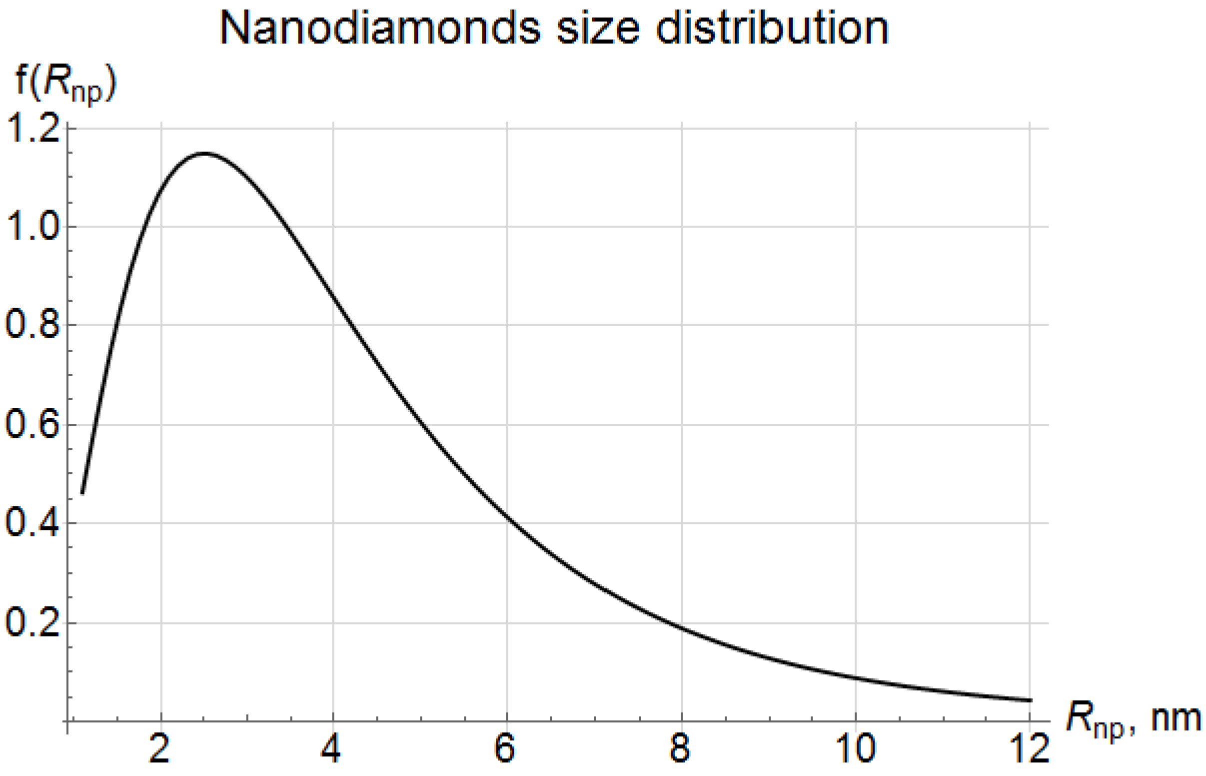


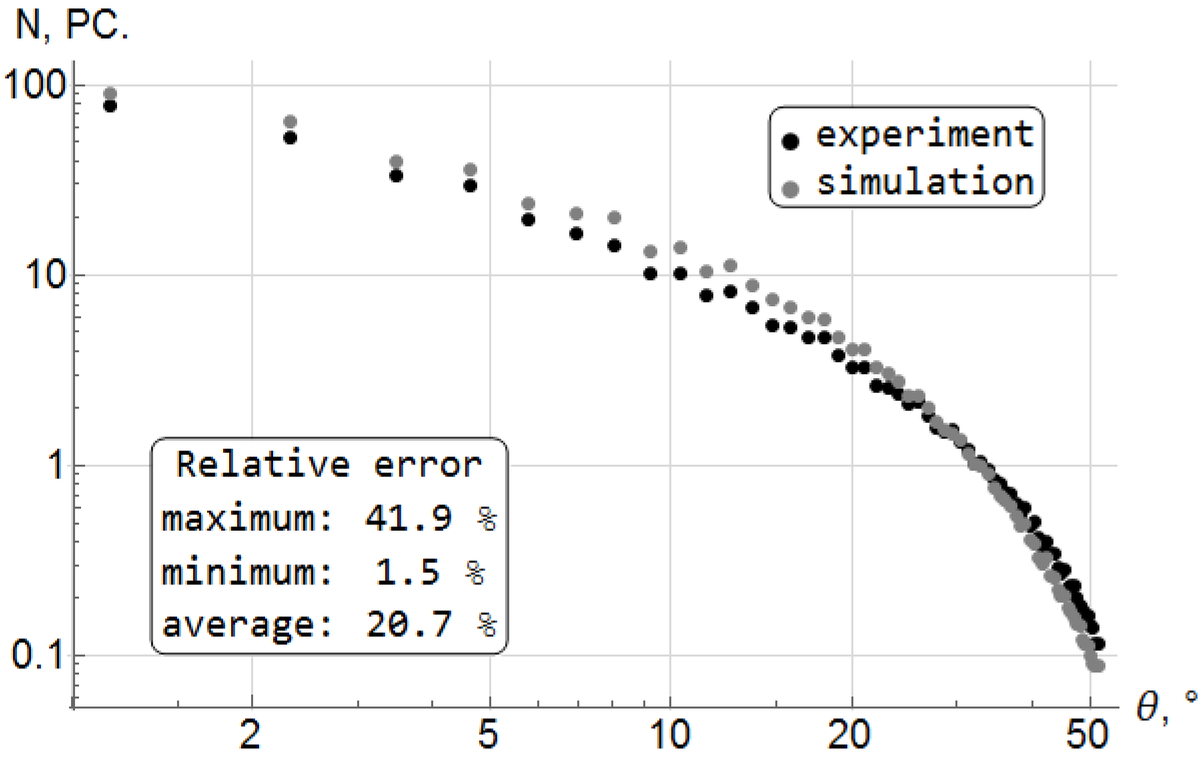
This calibration measurement must be used for a more accurate estimation of the phase composition, the size distribution of nanoparticles.

After the estimation is done the "nanotube" measurement will provide us the information about elemental composition.

Transmission of VCN

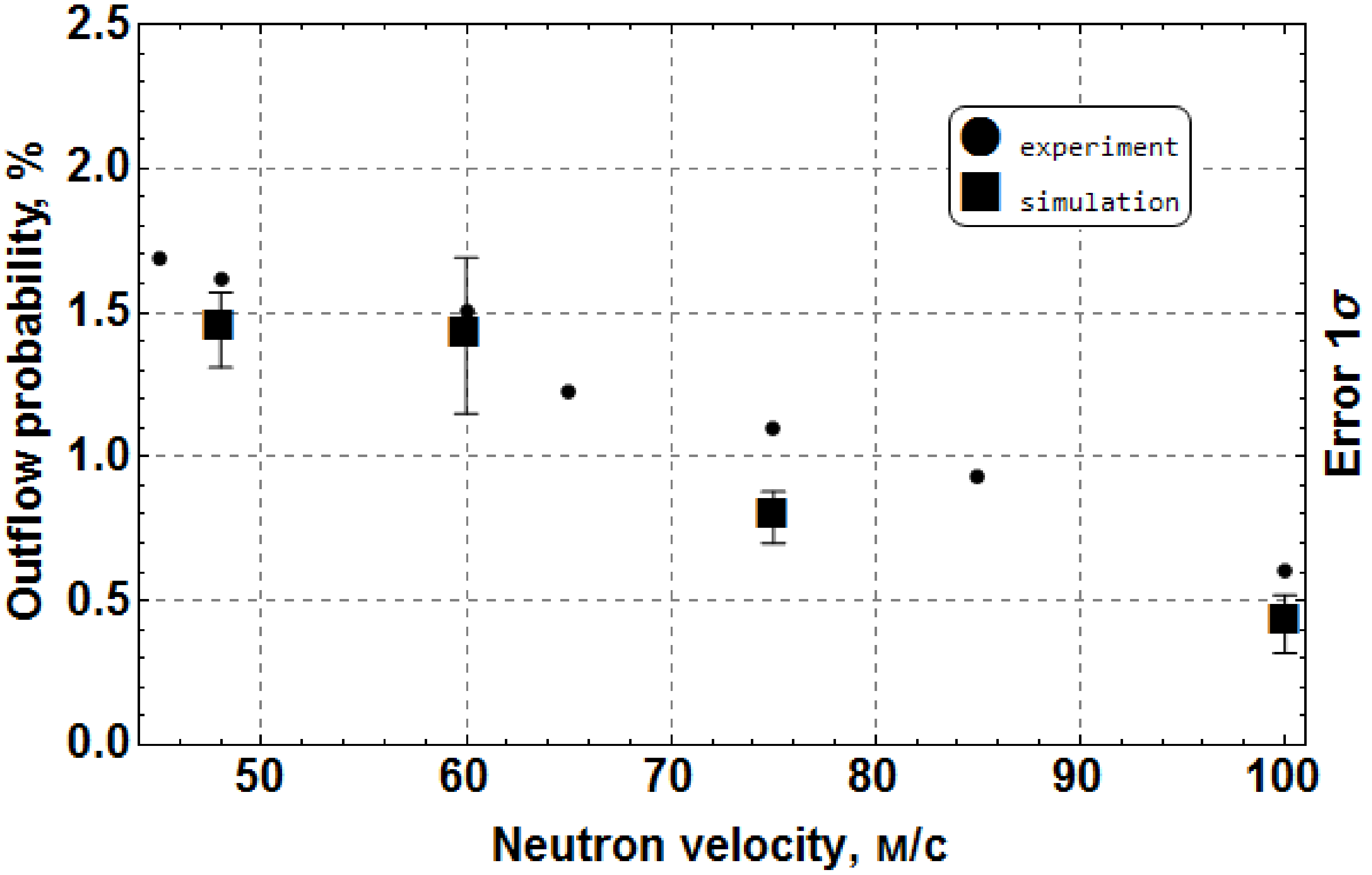
Interference effects are *conditionally* considered.
$M_{diamond}$ = 92 wt. %; shell thickness h = 6 Å.



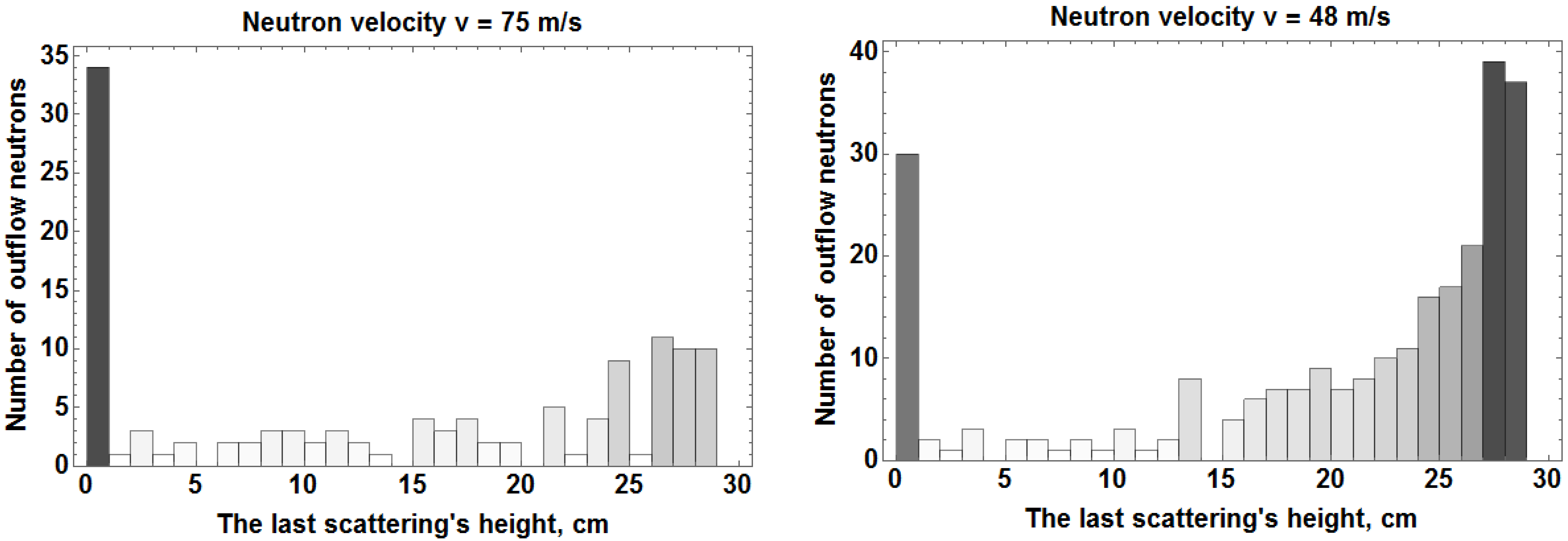


Extraction of VCN

The last result for $M_N = 3$ wt. %
Variation of the parameter value will continue.



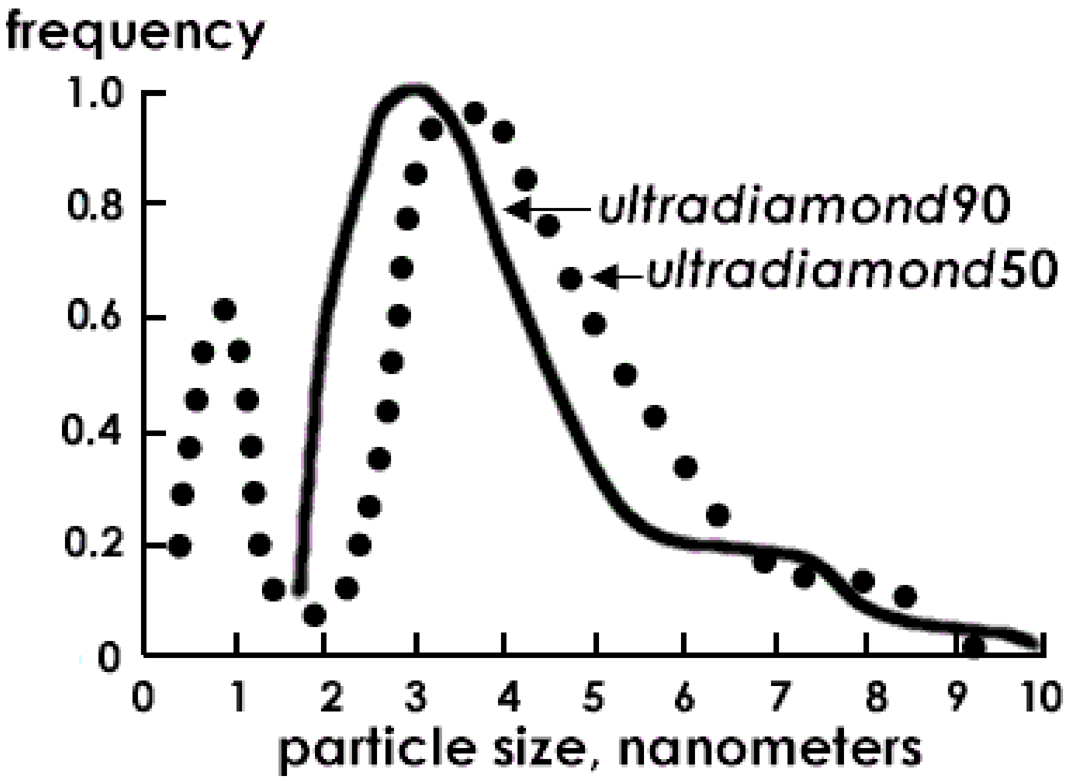
Extraction of VCN



Neutron outflow intensity as a function of the last scattering's height (cm).
N = 125 neutrons (left); N = 257 neutrons (right).

Interference effects accounting

Maybe it is reasonable to check a limiting case now: two, three or several nanoparticles are stick together.



Positive thoughts:

- only one more free parameter of the sticking;
- simulation via the "ultradiamond90" size distribution showed the best agreement with the experiment.

Conclusions

- We can simulate neutron transfer now:
  - none or a minimum number of free parameters - with sufficient error;
  - the presence of free parameters - with acceptable error.
- We have 2 workable physical models of non- and modified nanopowders.
- Software development continues; implemented algorithms might be imported into external simulation platforms (Geant4, etc.).
- We obtained a powerful tool for interpreting experimental data, planning future experiments, estimating and optimizing reflector parameters.

Thank you for your attention.

The “quasi-specular” reflection of CN and VCN

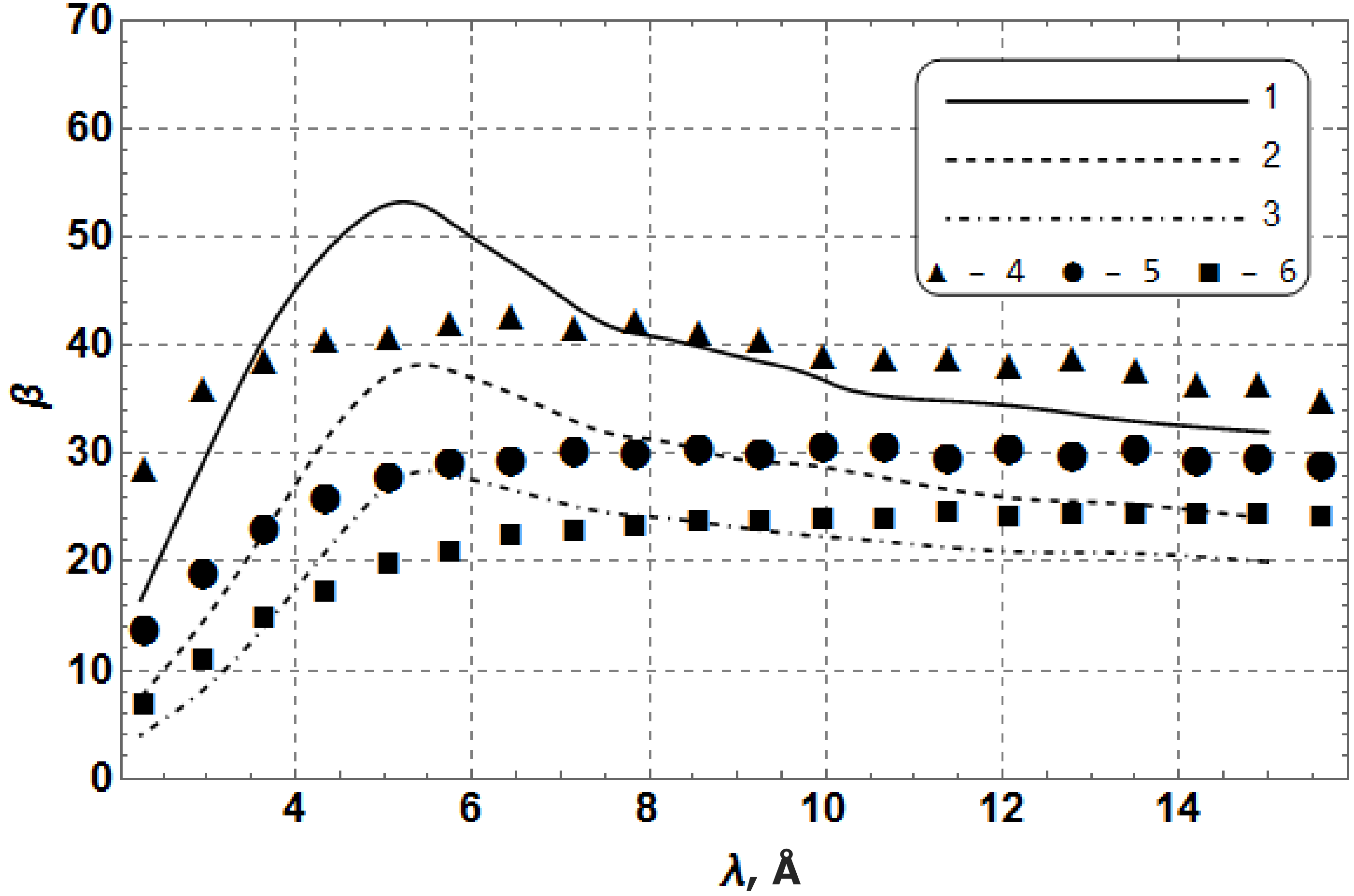


Fig.14. Probabilities of neutron scattering into the detector from the surface of a fluorinated diamond nanopowder.

Sliding angles of neutron falling:
1° (1), 2° (2), 3° (3).

The experimental data:
1° (4), 2° (5), 3° (6).

Fluorinated diamond nanopowder. The "quasi-specular" reflection of CN and VCN.

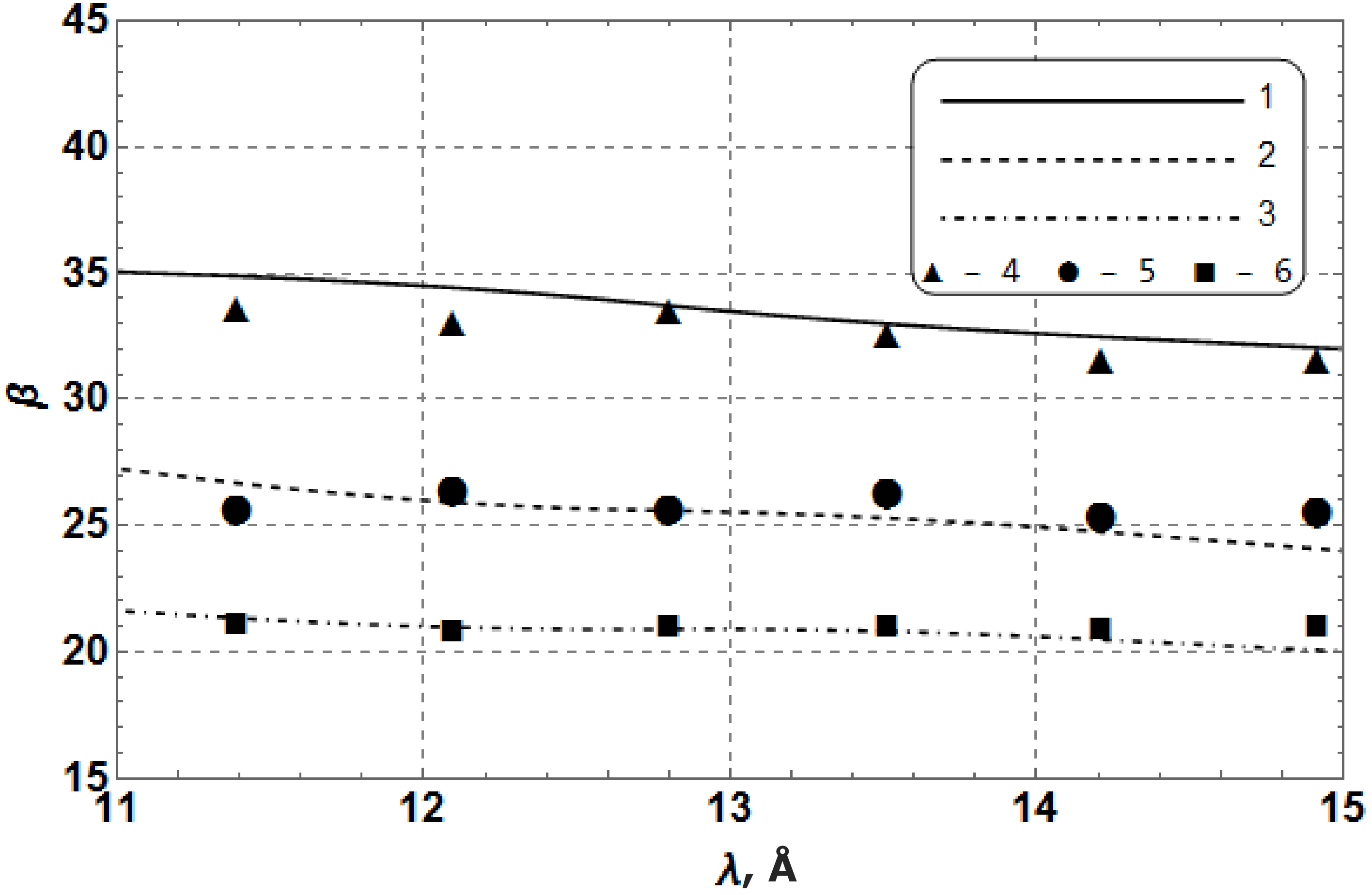


Fig.15. The target points β 1° (4), 2° (5), 3° (6) are renormalized by the index η=0.862.

Nezvanov A.Yu. Doctoral dissertation (2018)